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COMPUTING SEMIDEFINITE PROGRAMMING LOWER BOUNDS FOR THE (FRACTIONAL) CHROMATIC NUMBER VIA BLOCK-DIAGONALIZATION*

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Abstract. Recently we investigated in [*SIAM J. Optim.*, 19 (2008), pp. 572–591] hierarchies of semidefinite approximations for the chromatic number $\chi(G)$ of a graph G. In particular, we introduced two hierarchies of lower bounds: the "ψ"-hierarchy converging to the fractional chromatic number and the "Ψ"-hierarchy converging to the chromatic number of a graph. In both hierarchies the first order bounds are related to the Lovász theta number, while the second order bounds would already be too costly to compute for large graphs. As an alternative, relaxations of the second order bounds are proposed in [*SIAM J. Optim.*, 19 (2008), pp. 572–591]. We present here our experimental results with these relaxed bounds for Hamming graphs, Kneser graphs, and DIMACS benchmark graphs. Symmetry reduction plays a crucial role as it permits us to compute the bounds by using more compact semidefinite programs. In particular, for Hamming and Kneser graphs, we use the explicit block-diagonalization of the Terwilliger algebra given by Schrijver [*IEEE Trans. Inform. Theory*, 51 (2005), pp. 2859–2866]. Our numerical results indicate that the new bounds can be much stronger than the Lovász theta number. For some of the DIMACS instances we improve the best known lower bounds significantly.

Key words. chromatic number, Lovász theta number, semidefinite programming, Terwilliger algebra, Hamming graph, Kneser graph

AMS subject classifications. 05C15, 90C27, 90C22

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1. Introduction.

The chromatic number $\chi(G)$ of a graph G is the smallest number of colors needed to color the vertices of G so that no two adjacent vertices share the same color. Determining $\chi(G)$ is an NP-hard problem [14], and it is hard to approximate $\chi(G)$ within $|V(G)|^{1/14-\epsilon}$ for any $\epsilon > 0$ [1]. Finding a proper vertex coloring with a small number of colors is essential in many real-world applications. A lot of work has been done in order to develop efficient heuristics for this problem (see, e.g., [5]). Nevertheless, these methods can provide us only with upper bounds on the chromatic number. Lower bounds were mainly obtained by using linear programming [26, 27], critical subgraphs [8], and semidefinite programming (SDP) [9, 10, 11, 18, 28, 32]. The semidefinite approaches are based on computing (variations of) the well-known lower bound $\overline{\vartheta}(G) := \vartheta\left(\overline{G}\right)$, the theta number of the complementary graph, introduced by Lovász [24]. The theta number satisfies the "sandwich inequality":

$$\omega(G) \leq \overline{\vartheta}(G) \leq \chi(G),$$

and it can be computed to any arbitrary precision in polynomial time since it can be formulated via a semidefinite program of size $|V(G)|$. Here $\omega(G)$ is the clique number of G, defined as the maximum size of a clique (i.e., a set of pairwise adjacent nodes) in G, the stability number $\alpha(G) := \omega(\overline{G})$ of G being the maximum size of

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a stable set (i.e., a set of pairwise nonadjacent nodes) in G. The theta number has been strengthened towards the chromatic number by using nonnegativity [32], triangle inequalities [28], or some lift-and-project methods [11]. Computational results were reported in [9, 10, 11]. A common feature shared by all of these bounds is that they remain below the fractional chromatic number $\chi^*(G)$. Thus they are of little use when $\chi^*(G)$ is close to the clique number $\omega(G)$. In [17] the authors investigated another type of lift-and-project approach leading to a hierarchy of bounds converging to the chromatic number $\chi(G)$. We explore in the present follow-up paper the behavior of these bounds through experimental results on several classes of graphs.

The approach in [17] is based on the following reduction of Chvátal [6] of the chromatic number to the stability number:

$$\chi(G) \leq t \Longleftrightarrow \alpha(K_t \square G) = |V(G)|, \tag{1.1}$$

where $K_t \square G$ denotes the Cartesian product of K_t, the complete graph on t nodes, and the graph G. For a given graph parameter $\beta(\cdot)$ satisfying $\alpha(\cdot) \leq \beta(\cdot) \leq \overline{\chi}(\cdot)$, define the new graph parameter $\Psi_\beta(\cdot)$ by

$$\Psi_\beta(G) := \min_{t \in \mathbb{N}} t \ \text{ s.t. } \beta(K_t \square G) = |V(G)|. \tag{1.2}$$

As shown in [17], the operator Ψ is monotone nonincreasing and satisfies

$$\omega(G) = \Psi_{\overline{\chi}}(G) \leq \Psi_\beta(G) \leq \Psi_\alpha(G) = \chi(G) \text{ and } \Psi_\vartheta(G) = \left\lceil \overline{\vartheta}(G) \right\rceil. \tag{1.3}$$

In other words the operator Ψ transforms upper bounds for the stability number into lower bounds for the chromatic number. An interesting bound for $\alpha(\cdot)$ from the computational point of view is the graph parameter $\ell(\cdot)$ introduced by Laurent [21] as a relaxation of the second order bound in Lasserre's hierarchy for $\alpha(\cdot)$ (see [19, 21]). Two hierarchies for the chromatic number, related to Lasserre's hierarchy for $\alpha(\cdot)$, are studied in [17], as well as two bounds $\psi(\cdot)$ and $\Psi_\ell(\cdot)$ related to the parameter $\ell(\cdot)$. See section 2.2 for the precise definition of the parameters ℓ, ψ, and Ψ_ℓ.

In the present paper we investigate how to compute the bounds $\psi(\cdot)$ and $\Psi_\ell(\cdot)$ for Hamming graphs and for Kneser graphs. Coloring Hamming graphs is of interest, e.g., to the Borsuk problem (see [33]), and the chromatic number of Kneser graphs was computed in the celebrated paper [23] of Lovász by using topological methods; see, e.g., [25] for a study of topological lower bounds for the chromatic number. The Hamming graph $G = H(n, \mathcal{D})$ has node set $V(G) = \{0,1\}^n$, with an edge uv if the Hamming distance between u and v lies in the given set $\mathcal{D} \subseteq \{1, \dots, n\}$. For $n \geq 2r$, the Kneser graph $K(n,r)$ is the subgraph of $H(n, \{2r\})$ induced by the set of words $u \in \{0,1\}^n$ with weight $\sum_{i=1}^n u_i = r$. The Hamming graph has a large automorphism group which enables us to block-diagonalize and reformulate the programs for $\psi(G)$ and $\Psi_\ell(G)$ in such a way that they involve $O(n)$ matrices of size $O(n)$ (instead of $2^n = |V(G)|$). As a crucial ingredient we use the block-diagonalization for the Terwilliger algebra given by Schrijver [31]. We also use this technique, which was extended to constant-weight codes in [31], for computing the bound $\Psi_\ell(\cdot)$ for Kneser graphs. For Kneser graphs, the bound $\psi(\cdot)$ coincides with the fractional chromatic number (see section 4), but, as will be seen in Table 2, $\Psi_\ell(K(n,r))$ can go beyond the fractional chromatic number. We report experimental results for Hamming and Kneser graphs in Tables 1 and 2. For some instances, the parameter $\psi(G)$ improves substantially the theta number $\overline{\vartheta}(G)$, and adding nonnegativity may also help; moreover, while $\Psi_\ell(G)$ hardly improves upon $\psi(G)$ for Hamming graphs, it does give an improvement for Kneser graphs.

Finally we introduce a further variation $\psi_K(G)$ of our bounds (where K is a clique in G), which can be especially useful for graphs without apparent symmetries. By using a simple block-diagonalization argument, $\psi_K(G)$ can be formulated via a semidefinite program involving $|K|$ matrices of size $|V(G)|$ and one matrix of size $|V(G)|+1$. The bound $\psi_K(G)$ is bounded above by the fractional chromatic number $\chi^*(G)$. We report experimental results on some DIMACS benchmark instances. To the best of our knowledge, our lower bound improves the best known lower bound in the literature for several instances of DSJC and DSJR graphs, sometimes substantially. Moreover, for the two instances $G =$ DSJC125.9 and DSJR500.1c, we can determine the exact value of the chromatic number $\chi(G)$, since our lower bound matches the known upper bound for $\chi(G)$. This indicates that the bound ψ_K can be quite strong for random graphs, despite the fact that it remains below the fractional chromatic number. Moreover, we observed experimentally that adding nonnegativity constraints to the formulation of ψ_K does not help for the DSJC instances, which is similar to the observation made in [9] that strengthening the theta number with nonnegativity does not help for random graphs.

More details about the results of this paper can also be found in [16].

Contents of the paper. In section 2 we recall the definitions of the graph parameters $\ell(\cdot)$, $\psi(\cdot)$, and $\Psi_\ell(\cdot)$ and their main properties; we show how symmetry in the semidefinite programming formulations and in the graph can be exploited to (sometimes dramatically) reduce the sizes of the semidefinite programs defining these bounds. Section 3 is devoted to the computation of the bounds for Hamming graphs; we describe how to block-diagonalize the matrices in the semidefinite programs and report computational experiments. In section 4 we focus on the graph parameter $\Psi_\ell(\cdot)$ for Kneser graphs; we present the block-diagonalization of the matrices and conclude the section with computational results. We describe in section 5 the new lower bound $\psi_K(\cdot)$, which we test on some DIMACS benchmark graphs.

Notation. Given a graph $G = (V, E)$, $\overline{G}$ denotes its complementary graph whose edges are the pairs $uv \notin E(G)$ $(u, v \in V(G),\ u \neq v)$. Given a graph parameter $\beta(\cdot)$, $\overline{\beta}(\cdot)$ is the graph parameter defined by $\overline{\beta}(G) := \beta(\overline{G})$ for any graph G. For two graphs G and G', their Cartesian product $G \Box G'$ has node set $V(G) \times V(G')$, with two nodes uu', $vv' \in V(G) \times V(G')$ being adjacent in $G \Box G'$ if and only if ($u = v$ and $u'v' \in E(G')$) or ($uv \in E(G)$ and $u' = v'$). For an integer $t \geq 1$, K_t is the complete graph on t nodes. We also set $G_t = K_t \Box G$ as a shorthand notation for the Cartesian product of G and K_t.

Throughout, the letters $\mathbf{I}$, $\mathbf{J}$, and e denote, respectively, the identity matrix, the all-ones matrix, and the all-ones vector (of suitable size); $\mathbb{N}$ is the set of nonnegative integers. For matrices A and A' indexed, respectively, by $I \times J$ and $I' \times J'$, their tensor product $A \otimes A'$ is the matrix indexed by $(I \times I') \times (J \times J')$, with $(A \otimes A')_{(i,i'),(j,j')} := A_{i,j} B_{i',j'}$. Moreover, the notation $A \succeq 0$ means that A is a symmetric positive semidefinite matrix.

Given a finite set V, $\mathcal{P}(V)$ denotes the collection of all subsets of V. Given an integer r, set $\mathcal{P}_r(V) := \{I \in \mathcal{P}(V) \mid |I| \leq r\}$; in particular, $\mathcal{P}_1(V) = \{\emptyset, \{i\}\ (i \in V)\}$. Sometimes (e.g., when dealing with Hamming graphs) we deal with the collection $\mathcal{P}_1(V)$, where $V = \mathcal{P}(N)$, and $N = \{1, \ldots, n\}$; then $\mathcal{P}_1(V)$ contains $\emptyset$ (the empty subset of V) and $\{\emptyset\}$ (the singleton subset of V consisting of the empty subset of N). To avoid confusion we use the symbol $\mathbf{0}$ to denote the empty subset of V, so that $\mathcal{P}_1(V) = \{\mathbf{0}, \{i\}\ (i \in V)\}$. We sometimes identify $\mathcal{P}_1(V) \setminus \{\mathbf{0}\}$ with V; i.e., we write $\{i\}$ as i and $\{i,j\}$ as ij, and, given a vector $x \in \mathbb{R}^{\mathcal{P}(V)}$, we also set $x_i := x_{\{i\}}$, $x_{ij} := x_{\{i,j\}}$, $x_{ijk} := x_{\{i,j,k\}}$ (for $i,j,k \in V$), etc.

Let V be a finite set, and let $\mathcal{G}$ be a subgroup of $\mathrm{Sym}(V)$, the group of permutations of V, also denoted as $\mathrm{Sym}(n)$ if $|V| = n$. Then $\mathcal{G}$ acts on $\mathcal{P}(V)$ by letting $\sigma(I) := \{\sigma(i) \mid i \in I\}$ for $I \subseteq V$, $\sigma \in \mathcal{G}$. Moreover, $\mathcal{G}$ acts on vectors and matrices indexed by $\mathcal{P}_r(V)$, by letting $\sigma(x) := (x_{\sigma(I)})_{I \in \mathcal{P}_r(V)}$, $\sigma(M) := (M_{\sigma(I),\sigma(J)})_{I,J \in \mathcal{P}_r(V)}$ for $x \in \mathbb{R}^{\mathcal{P}_r(V)}$, $M \in \mathbb{R}^{\mathcal{P}_r(V) \times \mathcal{P}_r(V)}$, and $\sigma \in \mathcal{G}$. One says that M is invariant under the action of $\mathcal{G}$ if $\sigma(M) = M$ for all $\sigma \in \mathcal{G}$; then the matrix $\frac{1}{|\mathcal{G}|!} \sum_{\sigma \in \mathcal{G}} \sigma(M)$, the "symmetrization" of M obtained by applying the Reynolds operator, is invariant under the action of $\mathcal{G}$. The analogue statement holds for vectors. A semidefinite program is said to be invariant under the action of $\mathcal{G}$ if, for any feasible matrix X and any $\sigma \in \mathcal{G}$, the matrix $\sigma(X)$ is again feasible with the same objective value; then the optimum value of the program remains unchanged if we restrict to invariant feasible solutions, and, in particular, there is an invariant optimal solution.

The automorphism group $\mathrm{Aut}(G)$ of a graph $G = (V,E)$ consists of all $\sigma \in \mathrm{Sym}(V)$ preserving the set of edges. G is said to be vertex-transitive when, given any two nodes $i,j \in V$, there exists $\sigma \in \mathrm{Aut}(G)$, for which $\sigma(i) = j$. For instance, for the graph $G_t = K_t \square G$, $\mathrm{Sym}(t) \times \mathrm{Aut}(G) \subseteq \mathrm{Aut}(G_t)$, where $(\tau,\sigma) \in \mathrm{Sym}(t) \times \mathrm{Aut}(G)$ acts on $V(G_t)$ (and thus on $\mathcal{P}_r(V(G_t))$ for $r \in \mathbb{N}$) by $(\tau,\sigma)(p,i) = (\tau(p),\sigma(i))$ for $(p,i) \in V(K_t) \times V(G)$. We will deal in this paper with semidefinite programs involving matrices indexed by $\mathcal{P}_r(V(G_t))$, which are invariant under this action of $\mathrm{Sym}(t) \times \mathrm{Aut}(G)$.

2. Graph parameters.

2.1. Classic bounds. We recall here some classic bounds for the chromatic number $\chi(G)$ of a graph $G = (V,E)$. Throughout section 2, $V = V(G)$ is the node set of graph G and $n := |V(G)|$. (For details see, e.g., [17, 22, 30].)

- The *fractional chromatic number of* G:

$$\chi^*(G) := \max\ e^T x \ \text{ s.t. } \sum_{i \in S} x_i \le 1 \ (S \text{ stable}), \quad x \in \mathbb{R}^V_+. \tag{2.1}$$

It is well known (and easy to verify) that $\omega(G) \le \chi^*(G) \le \chi(G)$, and

$$\alpha(G)\chi^*(G) \ge |V(G)| \ \text{ with equality when } G \text{ is vertex-transitive.} \tag{2.2}$$

- *Lovász's theta number* (introduced in [24]):

$$\begin{aligned} \overline{\vartheta}(G) = \vartheta(\overline{G}) := \quad \max \quad & e^T Y e \\ \text{s.t.} \quad & \sum_{i \in V} Y_{ii} = 1, \\ & Y_{ij} = 0 \ \ (ij \in E(\overline{G})), \\ & Y \succeq 0, \end{aligned} \tag{2.3}$$

where Y is a symmetric matrix indexed by V. For a later purpose we recall the following equivalent formulation (cf., e.g., [15, Theorem 9.3.12]):

$$\begin{aligned} \overline{\vartheta}(G) = \quad \min \quad & X_{\mathbf{00}} \\ \text{s.t.} \quad & X_{ii} = X_{\mathbf{0}i} \ (i \in V), \\ & X_{ij} = 0 \ (ij \in E(G)), \\ & X \succeq 0, \end{aligned} \tag{2.4}$$

where the matrix variable X is indexed by the set $\mathcal{P}_1(V) = V \cup \{\mathbf{0}\}$. Lovász [24] proved the following analogue of (2.2) for the pair $(\vartheta, \overline{\vartheta})$:

$$\vartheta(G)\overline{\vartheta}(G) \geq |V(G)| \text{ with equality when } G \text{ is vertex-transitive.} \tag{2.5}$$

• *Szegedy's number* was first defined in [32]. We present the following equivalent formulation from [17]:

$$\begin{array}{rll} \overline{\vartheta^+}(G) = \vartheta^+(\overline{G}) = & \min & X_{\mathbf{00}} \\ & \text{s.t.} & X_{ii} = X_{\mathbf{0}i} \ (i \in V), \\ & & X_{ij} = 0 \ (ij \in E(G)), \\ & & X \geq 0, \ X \succeq 0. \end{array} \tag{2.6}$$

The above parameters satisfy

$$\omega(G) \leq \overline{\vartheta}(G) \leq \overline{\vartheta^+}(G) \leq \chi^*(G) \leq \chi(G).$$

2.2. The bounds $\boldsymbol{\ell}$, $\boldsymbol{\psi}$, and $\boldsymbol{\Psi_\ell}$. We review here the graph parameters $\ell(\cdot)$ proposed in [21] and $\psi(\cdot)$ and $\Psi_\ell(\cdot)$ proposed in [17]; for details see also [16]. For a subset $S \subseteq V$ and an integer $r \geq 1$, define the vectors $\chi^S \in \{0,1\}^V$, with ith entry 1 if and only if $i \in S$ (for $i \in V$), and $\chi^{S,r} \in \{0,1\}^{\mathcal{P}_r(V)}$, with Ith entry 1 if and only if $I \subseteq S$ (for $I \in \mathcal{P}_r(V)$). Given a vector $x = (x_I)_{I \in \mathcal{P}_{2r}(V)}$, consider the matrix:

$$M_r(x) := (x_{I \cup J})_{I, J \in \mathcal{P}_r(V)}$$

known as the *(combinatorial) moment matrix* of x of order r. Consider the programs:

$$\text{las}^{(r)}(G) := \max \sum_{i \in V} x_i \ \text{ s.t. } M_r(x) \succeq 0, \ x_{\mathbf{0}} = 1, \ x_{ij} = 0 \ (ij \in E), \tag{2.7}$$

$$\psi^{(r)}(G) := \min \ t \ \text{ s.t. } M_r(x) \succeq 0, \ x_{\mathbf{0}} = t, \, x_i = 1 \, (i \in V), \ x_{ij} = 0 \ (ij \in E), \tag{2.8}$$

where the variable x is indexed by $\mathcal{P}_{2r}(V)$. Note that the variable t can be avoided in (2.8) by replacing t by $x_{\mathbf{0}}$ in the objective function. We choose this formulation to emphasize the analogy with the formulations (2.13), (2.17), and (5.1) below. The above two programs were studied, respectively, in [19, 20] and in [17]. In particular, the following holds:

$$\alpha(G) = \text{las}^{(\alpha(G))} \leq \cdots \leq \text{las}^{(r+1)}(G) \leq \text{las}^{(r)}(G) \leq \cdots \leq \text{las}^{(1)}(G) = \vartheta(G), \tag{2.9}$$

$$\vartheta(\overline{G}) = \psi^{(1)}(G) \leq \cdots \leq \psi^{(r)}(G) \leq \psi^{(r+1)}(G) \leq \cdots \leq \psi^{(\alpha(G))}(G) = \chi^*(G), \tag{2.10}$$

$$\psi^{(r)}(G)\text{las}^{(r)}(G) \geq |V(G)| \text{ with equality if } G \text{ is vertex-transitive.} \tag{2.11}$$

Thus the parameters $\text{las}^{(r)}(G)$ (for $r = 1, \ldots, \alpha(G)$) create a hierarchy of upper bounds for the stability number, while the parameters $\psi^{(r)}(G)$ create a hierarchy of lower bounds for the fractional coloring number. Theoretically, the parameters $\text{las}^{(r)}(G)$ and $\psi^{(r)}(G)$ can be computed to any precision in polynomial time for fixed r, since the semidefinite programs (2.7) and (2.8) involve matrices of size $O(n^r)$. On the other hand, in practice, we are not able to compute $\text{las}^{(2)}(G)$ or $\psi^{(2)}(G)$ for "interesting" graphs, that is, for graphs of reasonably large size. For this reason some variations of the parameters $\text{las}^{(2)}(G)$ and $\psi^{(2)}(G)$ were proposed in [17, 21]. The idea is to consider, instead of the full moment matrix of order 2, a number of principal submatrices of it. Given $h \in V$, let $M_2(h;x)$ denote the principal submatrix of $M_2(x)$ indexed by the subset $\mathcal{P}_1(V) \cup \{\{h,i\} \mid i \in V\}$ of $\mathcal{P}_2(V)$. Thus in order to define the matrices $M_2(h;x)$ for all $h \in V$, one needs only the components of x indexed by $\mathcal{P}_3(V)$. Following [17, 21], define the upper bound for the stability number $\alpha(G)$:

$$\ell(G) := \max \sum_{i \in V} x_i \ \text{ s.t. } M_2(h;x) \succeq 0 \ (h \in V),\ x_{\mathbf{0}} = 1,\ x_{ij} = 0 \ (ij \in E(G)), \tag{2.12}$$

and the lower bound for the fractional coloring number $\chi^*(G)$:

$$\psi(G) := \min\ t \ \text{ s.t. } \begin{array}{l} M_2(h;x) \succeq 0 \ (h \in V),\ x_{ij} = 0 \ (ij \in E(G)), \\ x_{\mathbf{0}} = t,\ x_i = 1 \ (i \in V), \end{array} \tag{2.13}$$

where the variable x is indexed by $\mathcal{P}_3(V)$. For the parameter $\ell(G)$ we have (see [21])

$$\alpha(G) \le \mathrm{las}^{(2)}(G) \le \ell(G) \le \mathrm{las}^{(1)}(G) = \vartheta(G) \le \overline{\chi}(G), \tag{2.14}$$

while $\psi(G)$ satisfies (see [17])

$$\overline{\vartheta^{+}}(G) \le \psi(G) \le \psi^{(2)}(G). \tag{2.15}$$

They also satisfy an inequality similar to (2.11), namely,

$$\psi(G)\ell(G) \ge |V(G)| \text{ with equality if } G \text{ is vertex-transitive.} \tag{2.16}$$

As $\alpha(\cdot) \le \ell(\cdot) \le \overline{\chi}(\cdot)$ (by (2.14)), we can apply the operator Ψ from (1.2) to $\ell(\cdot)$ and obtain the lower bound $\Psi_\ell(G)$ for $\chi(G)$, defined as

$$\Psi_\ell(G) = \min_{t \in \mathbb{N}}\ t \ \text{ s.t. } \ell(G_t) = n. \tag{2.17}$$

The parameter $\ell(G_t)$ is defined via the program

$$\ell(G_t) = \max \sum_{u \in V(G_t)} y_u \ \text{ s.t. } \begin{array}{l} M_2(u;y) \succeq 0 \ (u \in V(G_t)), \\ \\ y_{\mathbf{0}} = 1,\ y_{uv} = 0 \ (uv \in E(G_t)), \end{array} \tag{2.18}$$

where the variable y is indexed by $\mathcal{P}_3(V(G_t))$. (Recall that $G_t = K_t \square G$.) Finally, the two parameters $\psi(G)$ and $\Psi_\ell(G)$ were compared in [17], where the following relation is shown:

$$\overline{\vartheta}(G) \le \psi(G) \le \Psi_\ell(G) \le \chi(G). \tag{2.19}$$

Let us finally note that one can easily strengthen the bounds $\ell(G)$, $\psi(G)$, and $\Psi_\ell(G)$, e.g., by requiring nonnegativity[1] of the variables. Let $\ell_{\ge 0}(G)$ (resp., $\psi_{\ge 0}(G)$) denote the variation of $\ell(G)$ (resp., $\psi(G)$) obtained by adding the condition $x \ge 0$ to

[1] Note, however, that the condition $x_{ij} \ge 0 \ \ \forall i,j \in V$ already automatically holds in (2.12) and (2.13), since it is implied by $M_2(h;x) \succeq 0 \ \forall h \in V$ (as x_{hi} occurs as a diagonal entry of $M_2(h;x)$). Analogously, $y_{uv} \ge 0 \ \ \forall u,v \in V(G_t)$ automatically holds in (2.18).

(2.12) (resp., (2.13)); we have again $\psi_{\geq 0}(G)\ell_{\geq 0}(G) = |V(G)|$ when G is vertex-transitive. Define accordingly $\Psi_{\ell_{\geq 0}}(G)$, which amounts to requiring $y \geq 0$ in (2.18).

2.3. Exploiting symmetry to compute the bounds ℓ, ψ, and Ψ_ℓ. We group here some observations about the complexity of computing the graph parameters $\ell(\cdot)$, $\psi(\cdot)$, and $\Psi_\ell(\cdot)$. We show how one can exploit symmetry, present in the structure of the matrices involved in the programs defining the parameters or in the graph instance, in order to reduce the size of the programs. This symmetry reduction is a crucial step as it allows reformulating the parameters via more compact programs. In this way we will be able to compute the graph parameters for certain large graphs (with as many as 2^{20} nodes for certain Hamming graphs), a task that would obviously be out of reach without applying this symmetry reduction.

We begin with observing that the matrix $M_2(h;x)$, used in definitions (2.12) and (2.13), has a special block structure, whose symmetry can be exploited to "block-diagonalize" it. Recall that $M_2(h;x)$ is indexed by the set $\mathcal{P}_1(V) \cup \{\{h,i\} \mid i \in V\} = \{\mathbf{0}\} \cup \{\{i\} \mid i \in V\} \cup \{\{h,i\} \mid i \in V\}$. Here we keep the two occurrences of the singleton $\{h\}$ in the index set, occurring first as $\{i\}$ for $i = h$ and second as $\{i,h\}$ for $i = h$. Thus, the index set of $M_2(h;x)$ is partitioned into $\{\mathbf{0}\}$ and two copies of V.

LEMMA 2.1. *With respect to this partition of its index set, the matrix $M_2(h;x)$ has the block form:*

$$M_2(h;x) = \begin{pmatrix} a & c^T & d^T \\ c & C & D \\ d & D & D \end{pmatrix}, \tag{2.20}$$

where $a = x_{\mathbf{0}}$, $c_i = x_i$, $d_i = x_{hi}$ $(i \in V)$, $C_{ij} = x_{ij}$, and $D_{ij} = x_{hij}$ $(i,j \in V)$. Then

$$M_2(h;x) \succeq 0 \Longleftrightarrow \begin{pmatrix} a - c_h & c^T - d^T \\ c - d & C - D \end{pmatrix} \succeq 0 \quad \textit{and} \quad D \succeq 0. \tag{2.21}$$

Proof. The form (2.20) follows directly from the definition of $M_2(h;x)$. To show (2.21), observe that the row of $M_2(h;x)$ indexed by $\{h\}$ has the form (c_h, d^T, d^T). Indeed, for $i,j \in V$, $C_{ij} = x_{\{i,j\}}$, $D_{ij} = x_{\{h,i,j\}}$, $c_j = x_j$, and $d_j = x_{\{h,j\}}$, implying that $C_{hj} = D_{hj} = d_j$. As in [21], we perform some row/column manipulation on $M_2(h;x)$ to show (2.21). Say the second row/column of $M_2(h;x)$ is indexed by $\{h\}$, i.e., h comes first when listing the elements of V. Then

$$U_1^T M_2(h;x) U_1 = \begin{pmatrix} a - c_h & c^T - d^T & 0 \\ c - d & C & D \\ 0 & D & D \end{pmatrix}, \quad \text{setting } U_1 := \begin{pmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \mathbf{I} \end{pmatrix},$$

where $\mathbf{I}$ is the identity matrix of order $2n-1$ $(n = |V|)$. Next,

$$U_2^T (U_1^T M_2(h;x) U_1) U_2 = \begin{pmatrix} a - c_h & c^T - d^T & 0 \\ c - d & C - D & 0 \\ 0 & 0 & D \end{pmatrix}, \quad \text{setting } U_2 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & \mathbf{I} & 0 \\ 0 & -\mathbf{I} & \mathbf{I} \end{pmatrix},$$

where $\mathbf{I}$ has order n. ◻

Hence, in (2.12) and (2.13), we may replace each constraint $M_2(h;x) \succeq 0$ (which involves a matrix of size $2n+1$) by two constraints involving matrices of sizes $n+1$ and n.

We now consider symmetries present in the graph instance G. Observe that the program (2.12) (or (2.13)) is invariant under the action of $\mathrm{Aut}(G)$. Hence one may assume that the variable x is invariant under the action of $\mathrm{Aut}(G)$. Therefore, when G is vertex-transitive, it suffices to require the condition $M_2(h;x) \succeq 0$ for *one* choice of $h \in V$ (instead of for *all* $h \in V$), and thus $\ell(G)$ and $\psi(G)$ can be computed via a semidefinite program involving two linear matrix inequality (LMIs) matrices of sizes $n+1$, n and with $O(n^2)$ variables.

We now turn to the graph parameter $\Psi_\ell(G)$. In order to determine $\Psi_\ell(G)$, we need to compute the parameter $\ell(G_t) = \ell(K_t \square G)$ from (2.18) (for several queries of $t \in \mathbb{N}$). As was just observed above, the program defining $\ell(G_t)$ is invariant under the action of $\mathrm{Aut}(G_t)$ thus in particular under the action of $\mathrm{Sym}(t) \times \mathrm{Aut}(G)$ or simply of $\mathrm{Sym}(t)$. In particular, in program (2.18), one may assume that y is invariant under the action of $\mathrm{Sym}(t)$. Moreover, it suffices to require the condition $M_2(u;y) \succeq 0$ for all $u \in V_1$ instead of for all $u \in V(G_t)$; here $V_1 = \{1i \mid i \in V\}$ denotes the "first layer" of the node set $V(G_t) = \{pi \mid p = 1, \ldots, t,\ i \in V\}$ of G_t. Furthermore, when G is vertex-transitive, it suffices to require $M_2(u;y) \succeq 0$ for *one* choice of $u \in V_1$ instead of for *all* $u \in V_1$.

We now show, by using the invariance of y under the action of $\mathrm{Sym}(t)$, that the matrix $M_2(u;y)$ has a special block structure, whose symmetry can be used to block-diagonalize it. To begin with, with respect to the partition $\{\mathbf{0}\} \cup \{\{v\} \mid v \in V(G_t)\} \cup \{\{u,v\} \mid v \in V(G_t)\}$ of its index set, the matrix $M_2(u;y)$ has the block form shown in (2.20) with a, c, d, C, and D being now defined in terms of y (instead of x). In view of (2.21), we have

$$M_2(u;y) \succeq 0 \Longleftrightarrow \begin{pmatrix} y_{\mathbf{0}} - y_u & c^T - d^T \\ c - d & C - D \end{pmatrix} \succeq 0 \ \text{ and } \ D \succeq 0. \tag{2.22}$$

Next we observe that the invariance of y under $\mathrm{Sym}(t)$ implies a special block structure for the matrices C and D.

LEMMA 2.2. *Consider the partition $V(G_t) = V_1 \cup \cdots \cup V_t$ of the node set of graph G_t, where $V_p := \{pi \mid i \in V\}$ for $p = 1, \ldots, t$. With respect to this partition, the matrices C and D have the block form:*

$$C = \begin{pmatrix} A^1 & A^2 & \cdots & A^2 \\ A^2 & A^1 & \cdots & A^2 \\ \vdots & \vdots & \ddots & \vdots \\ A^2 & \cdots & \cdots & A^1 \end{pmatrix}, \qquad D = \begin{pmatrix} B^1 & B^2 & B^2 & \cdots & B^2 \\ (B^2)^T & B^3 & B^4 & \cdots & B^4 \\ (B^2)^T & B^4 & B^3 & \cdots & B^4 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ (B^2)^T & B^4 & \cdots & \cdots & B^3 \end{pmatrix}, \tag{2.23}$$

where[2] $A^1, \ldots, B^4 \in \mathbb{R}^{n \times n}$. *Moreover, by setting $a_1 := \mathrm{diag}(A^1)$, $b_1 := \mathrm{diag}(B^1)$, and $b_3 := \mathrm{diag}(B^3)$, we have $c = [a_1^T, \ldots, a_1^T]^T$ and $d = [b_1^T\, b_3^T\, b_3^T, \ldots, b_3^T]^T$.*

Proof. Consider $i, j \in V$ and $p, q, p', q' \in \{1, \ldots, t\}$, with $p = q$ if and only if $p' = q'$. Then $C_{pi,qj} = y_{\{pi,qj\}} = y_{\{p'i,q'j\}} = C_{p'i,q'j}$; indeed, as there exists $\sigma \in \mathrm{Sym}(t)$ mapping $\{p,q\}$ to $\{p',q'\}$, the equality $y_{\{pi,qj\}} = y_{\{p'i,q'j\}}$ follows from the fact that y is invariant under the action of $\mathrm{Sym}(t)$. This shows that C has the form indicated in (2.23); the argument is analogous for matrix D. ∎

[2] Here A^i or B^i should not be interpreted as powers of A or B, as i is not an exponent but just an upper index.

To fix ideas, set $u = 1h \in V_1$ (where $h \in V$ is a given node of G). Then the entries of $A^1, \ldots, B^4$ are given by

$$\begin{gathered} A^1_{ij} = y_{\{1i,1j\}},\ A^2_{ij} = y_{\{1i,2j\}},\ B^1_{ij} = y_{\{1i,1h,1j\}}, \\ B^2_{ij} = y_{\{1i,1h,2j\}},\ B^3_{ij} = y_{\{2i,1h,2j\}},\ B^4_{ij} = y_{\{2i,1h,3j\}} \end{gathered} \tag{2.24}$$

for $i, j \in V$. (Recall that $y_{\{1i,1j\}} = y_{\{pi,pj\}}$, $y_{\{1i,2j\}} = y_{\{pi,qj\}}$, and $y_{\{1i,2j,3h\}} = y_{\{pi,qj,rh\}}$ for any distinct $p, q, r \in \{1, \ldots, t\}$ since y is invariant under the action of $\mathrm{Sym}(t)$.) Moreover, the edge constraints $y_{uv} = 0$ (for $uv \in E(G_t)$) in (2.18) can be reformulated as

$$\begin{aligned} &A^1_{ij} = 0 \ \text{ if } \ ij \in E(G), \\ &B^1_{ij} = 0 \ \text{ if } \ \{i, j, h\} \text{ contains an edge of } G, \\ &B^2_{ij} = 0 \ \text{ if } \ hi \in E(G) \text{ or } j \in \{i, h\}, \\ &B^3_{ij} = 0 \ \text{ if } \ ij \in E(G) \text{ or if } h \in \{i, j\}, \\ &B^4_{ij} = 0 \ \text{ if } \ h \in \{i, j\}, \\ &\mathrm{diag}(A^2) = \mathrm{diag}(B^2) = \mathrm{diag}(B^4) = 0 \end{aligned} \tag{2.25}$$

for distinct $i, j \in V$.

The next lemma indicates how one can further block-diagonalize the two matrices appearing at the right-hand side of the equivalence in (2.22).

LEMMA 2.3. *We have*

$$D \succeq 0 \Longleftrightarrow \begin{pmatrix} B^1 & (t-1)B^2 \\ (t-1)(B^2)^T & (t-1)B^3 + (t-1)(t-2)B^4 \end{pmatrix},\ B^3 - B^4 \succeq 0.$$

Moreover,

$$\begin{pmatrix} y_{\mathbf{0}} - y_u & c^T - d^T \\ c - d & C - D \end{pmatrix} \succeq 0 \Longleftrightarrow A^1 - B^3 - A^2 + B^4 \succeq 0 \quad \textit{and}$$

$$\begin{pmatrix} y_{\mathbf{0}} - y_u & a_1^T - b_1^T & (t-1)(a_1^T - b_3^T) \\ & A^1 - B^1 & (t-1)(A^2 - B^2) \\ & & (t-1)(A^1 - B^3) + (t-1)(t-2)(A^2 - B^4) \end{pmatrix} \succeq 0.$$

(We wrote only the upper triangular part in the above (symmetric) matrix.)

Proof. Consider the orthogonal matrices

$$M := \begin{pmatrix} \mathbf{I} & 0 \\ 0 & U_{t-1} \end{pmatrix}, \qquad N := \begin{pmatrix} 1 & 0 \\ 0 & M \end{pmatrix},$$

where $\mathbf{I}$ is the identity matrix of order n and U_{t-1} is defined as follows. U_{t-1} is a $(t-1) \times (t-1)$ block matrix where, for $p, q = 1, \ldots, t-1$, its (p, q)th block U^{pq}_{t-1} is the $n \times n$ matrix defined as

$$U^{pq}_{t-1} := \begin{cases} \frac{1}{\sqrt{t-1}}\mathbf{I} & \text{if } p = 1 \text{ or } q = 1, \\ \left(\frac{1}{\sqrt{t-1}+t-1} - 1\right)\mathbf{I} & \text{if } p = q \geq 2, \\ \frac{1}{\sqrt{t-1}+t-1}\mathbf{I} & \text{otherwise.} \end{cases} \tag{2.26}$$

Notice that U_{t-1} is symmetric and orthogonal, i.e., $U_{t-1}(U_{t-1})^T = \mathbf{I}$. A simple calculation shows that

$$MDM = \begin{pmatrix} B^1 & \sqrt{t-1}B^2 & 0 & \dots & 0 \\ \sqrt{t-1}(B_2)^T & B^3+(t-2)B^4 & 0 & \dots & 0 \\ 0 & 0 & B^3-B^4 & & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & B^3-B^4 \end{pmatrix}.$$

The first assertion of the lemma now follows after multiplying the second row/column block by $\sqrt{t-1}$. Next we have

$$N\begin{pmatrix} y_{\mathbf{0}}-y_u & c^T-d^T \\ c-d & C-D \end{pmatrix} N = \begin{pmatrix} y_{\mathbf{0}}-y_u & (c-d)^T M \\ M(c-d) & M(C-D)M \end{pmatrix}.$$

As the matrix $C-D$ has the same type of block shape as D, we deduce from the above that $M(C-D)M$ is block-diagonal. More precisely, the first diagonal block has the form

$$\begin{pmatrix} A^1-B^1 & \sqrt{t-1}(A^2-B^2) \\ \sqrt{t-1}(A^2-B^2)^T & (A^1-B^3)+(t-2)(A^2-B^4) \end{pmatrix},$$

and the remaining $t-2$ diagonal blocks are all equal to $A^1-B^3-A^2+B^4$. One can moreover verify that $(c-d)^T M = \left(a_1^T-b_1^T, \sqrt{t-1}(a_1^T-b_3^T), 0\dots 0\right)$. From this follows the second assertion of the lemma. □

In summary, we have obtained the following more compact semidefinite program for the parameter $\ell(G_t)$:

(2.27)

$$\begin{aligned} \ell(G_t) = \ \max\ te^T a_1 \ \text{ s.t. } & a_1 = \operatorname{diag}(A^1),\ b_1 = \operatorname{diag}(B^1),\ b_3 = \operatorname{diag}(B^3) \in \mathbb{R}^n, \\ & A^1, A^2, B^1, B^2, B^3, B^4 \in \mathbb{R}^{n\times n} \text{ satisfy (2.25) and} \\ & \begin{pmatrix} 1-(a_1)_h & a_1^T-b_1^T & (t-1)(a_1^T-b_3^T) \\ & A^1-B^1 & (t-1)(A^2-B^2) \\ & & (t-1)(A^1-B^3)+(t-1)(t-2)(A^2-B^4) \end{pmatrix} \succeq 0, \\ & \begin{pmatrix} B^1 & (t-1)B^2 \\ & (t-1)B^3+(t-1)(t-2)B^4 \end{pmatrix} \succeq 0, \\ & A^1-A^2-B^3+B^4 \succeq 0, \\ & B^3-B^4 \succeq 0. \end{aligned}$$

This formulation applies when G is vertex-transitive; here h is any fixed node of G. Hence $\Psi_\ell(G)$ can be obtained by computing $\ell(G_t)$ for $O(\log n)$ queries of the parameter t (see [17]) and the computation of each $\ell(G_t)$ is via an SDP involving four LMIs matrices of size $2n+1$, $2n$, n, and n, respectively. The above reductions obviously apply to the stronger bound $\Psi_{\ell_{\geq 0}}$ obtained by adding nonnegativity, i.e., by adding the constraints $A^1,\dots,B^4 \geq 0$ in (2.27).

3. Bounds for Hamming graphs. We indicate here how to compute the parameters $\psi(G)$ and $\Psi_\ell(G)$ when G is a Hamming graph. Given an integer $n \geq 1$ and $\mathcal{D} \subseteq N := \{1,\dots,n\}$, G is the graph $H(n,\mathcal{D})$ with node set $V(G) := \mathcal{P}(N)$ and with an edge (I,J) if $|I \triangle J| \in \mathcal{D}$ (for $I,J \in \mathcal{P}(N)$). Thus we now have $|V(G)| = 2^n$.

As G is vertex-transitive, we can use the program (2.27). As the program (2.27) involves matrices of size $O(2^n)$, it cannot be solved directly for interesting values of n. However, one can use the fact that the Hamming graph $G = H(n, \mathcal{D})$ has a large automorphism group for reducing the size of the matrices $A^1, \dots, B^4$ involved in the program (2.27). Each permutation $\sigma \in \mathrm{Sym}(n)$ induces an automorphism of G by letting $\sigma(I) := \{\sigma(i) \mid i \in I\}$ for $I \in \mathcal{P}(N)$, and, for any $K \in \mathcal{P}(N)$, the *switching mapping* s_K defined by $s_K(I) := I \triangle K$ (for $I \in \mathcal{P}(N)$) is also an automorphism of G. Then $\mathrm{Aut}(G) = \{\sigma s_K \mid \sigma \in \mathrm{Sym}(n),\ K \in \mathcal{P}(N)\}$ and $|\mathrm{Aut}(G)| = n!2^n$.

It turns out that the matrices $A^1, \dots, B^4$ appearing in (2.27) belong to the Terwilliger algebra of the Hamming graph. By using the explicit block-diagonalization of the Terwilliger algebra, presented by Schrijver [31], we are able to block-diagonalize the matrices in (2.27) which enables the computation of $\Psi_\ell(G)$ for $G = H(n, \mathcal{D})$ for n up to 20. We recall the details needed for our treatment in the next subsection.

3.1. The Terwilliger algebra. For $i, j, p = 0, \dots, n$, let $M_{i,j}^{p,n}$ denote the 0/1 matrix indexed by $\mathcal{P}(N)$ whose (I, J)th entry is 1 if $|I| = i$, $|J| = j$, and $|I \cap J| = p$ and equal to 0 otherwise. The set

$$\mathcal{A}_n := \left\{ \sum_{i,j,p=0}^{n} x_{i,j}^p M_{i,j}^{p,n} \mid x_{i,j}^p \in \mathbb{R} \right\}$$

is an algebra, known as the *Terwilliger algebra* of the Hamming graph. For $k = 0, \dots, n$, let M_k^n be the matrix indexed by $\mathcal{P}(N)$ whose (I, J)th entry is 1 if $|I \triangle J| = k$ and 0 otherwise. The set

$$\mathcal{B}_n := \left\{ \sum_{k=0}^{n} x_k M_k^n \mid x_k \in \mathbb{R} \right\}$$

is an algebra, known as the *Bose–Mesner algebra* of the Hamming graph. Obviously, $\mathcal{B}_n \subseteq \mathcal{A}_n$, since $M_k^n = \sum_{i,j,p \mid i+j-2p=k} M_{i,j}^{p,n}$. As is well known, $\mathcal{B}_n$ is a commutative algebra, and thus all matrices in $\mathcal{B}_n$ can be simultaneously diagonalized (cf. Delsarte [7]). The Terwilliger algebra is not commutative, and thus it cannot be diagonalized; however, it can be block-diagonalized, as explained in [31]. We recall the main result below.

Given integers $i, j, k, p = 0, \dots, n$, set

$$(3.1) \qquad \beta_{i,j,k}^{p,n} := \sum_{u=0}^{n} (-1)^{p-u} \binom{u}{p} \binom{n-2k}{n-k-u} \binom{n-k-u}{i-u} \binom{n-k-u}{j-u},$$

$$(3.2) \qquad \alpha_{i,j,k}^{p,n} := \beta_{i,j,k}^{p,n} \binom{n-2k}{i-k}^{-\frac{1}{2}} \binom{n-2k}{j-k}^{-\frac{1}{2}}.$$

THEOREM 3.1 (see [31]). *For a matrix $M = \sum_{i,j,p} M_{i,j}^{p,n} x_{i,j}^p$ in the Terwilliger algebra,*

$$(3.3) \qquad M \succeq 0 \Longleftrightarrow M_k := \left(\sum_p \alpha_{i,j,k}^{p,n} x_{i,j}^p \right)_{i,j=k}^{n-k} \succeq 0 \quad \text{for } k = 0, 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor.$$

To show this, Schrijver [31] constructs an orthogonal matrix U having the following property:

$$U^T M U = \begin{pmatrix} \widehat{M}_0 & 0 & \dots & 0 \\ 0 & \widehat{M}_1 & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & \widehat{M}_{\lfloor n/2 \rfloor} \end{pmatrix}, \quad \text{where } \widehat{M}_k = \begin{pmatrix} M_k & 0 & \dots & 0 \\ 0 & M_k & \dots & 0 \\ \vdots & \vdots & \ddots & 0 \\ 0 & 0 & \dots & M_k \end{pmatrix},$$

with block M_k being repeated $\binom{n}{k} - \binom{n}{k-1}$ times, for $k = 0, \dots, \lfloor n/2 \rfloor$.

The result extends to a block matrix whose blocks all lie in the Terwilliger algebra and which has a border of a special form. We state Lemma 3.2 for a 2×2 block matrix, but the analogous result holds obviously for any number of blocks.

LEMMA 3.2. *Let $A, B, C \in \mathcal{A}_n$, say, $A = \sum_{i,j,p} a_{i,j}^p M_{i,j}^{p,n}$, $B = \sum_{i,j,p} b_{i,j}^p M_{i,j}^{p,n}$, and $C = \sum_{i,j,p} c_{i,j}^p M_{i,j}^{p,n}$, and define accordingly*

$$A_k = \left(\sum_p \alpha_{i,j,k}^{p,n} a_{i,j}^p \right)_{i,j=k}^{n-k}, \; B_k = \left(\sum_p \alpha_{i,j,k}^{p,n} b_{i,j}^p \right)_{i,j=k}^{n-k}, \; C_k = \left(\sum_p \alpha_{i,j,k}^{p,n} c_{i,j}^p \right)_{i,j=k}^{n-k}.$$

Then

$$\begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \succeq 0 \iff \begin{pmatrix} A_k & B_k \\ B_k^T & C_k \end{pmatrix} \succeq 0 \;\forall k = 0, 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor.$$

Proof. The proof follows directly from the above by using the orthogonal matrix $\left(\begin{smallmatrix} U & 0 \\ 0 & U \end{smallmatrix}\right)$. □

LEMMA 3.3 (see Lemma 1 in [21]). *Let $M = \sum_{i,j,p=0}^n x_{i,j}^p M_{i,j}^{p,n} \in \mathcal{A}_n$, $c = \sum_{i=0}^n c_i \chi^i$, where $\chi^i \in \{0,1\}^{\mathcal{P}(N)}$ with $\chi_I^i = 1$ if $|I| = i$ (for $I \in \mathcal{P}(N)$), and $d \in \mathbb{R}$. Then*

$$\begin{pmatrix} d & c^T \\ c & M \end{pmatrix} \succeq 0 \iff \begin{cases} M_k \succeq 0 \;\; \text{for } k = 1, \dots, \left\lfloor \frac{n}{2} \right\rfloor, \\ \tilde{M}_0 := \begin{pmatrix} d & \tilde{c}^T \\ \tilde{c} & M_0 \end{pmatrix} \succeq 0 \end{cases}$$

after setting $\tilde{c}^T := (c_i \sqrt{\binom{n}{i}})_{i=0}^n$.

3.2. Compact formulation for $\psi(G)$ for Hamming graphs. As the graph $G = H(n, \mathcal{D})$ is vertex-transitive, we have $\psi(G) = \frac{2^n}{\ell(G)}$ by (2.16). It is shown in [21] how to compute the parameter $\ell(G)$ (when $\mathcal{D}$ is an interval $[1, d]$, but the reasoning is the same for any $\mathcal{D}$). The basic idea is that the matrix $M_2(h; x)$ appearing in (2.12) is a block matrix whose blocks lie in the Terwilliger algebra, and thus it can be block-diagonalized. We recall the details, directly for the parameter $\psi(G)$ from (2.13), as they will be useful for our treatment of the parameter $\Psi_\ell(G)$ in the next section.

Let x be feasible for the program (2.13). As G is vertex-transitive it suffices to require the condition $M_2(h; x) \succeq 0$ in (2.13) for *one* choice of $h \in V(G)$. Moreover, we may assume that the variable x is invariant under the action of the automorphism group of G. To fix ideas, let us choose the node $h := \emptyset$ of G (the empty subset of N). The matrix $M_2(\emptyset; x)$ has the block form

$$M_2(\emptyset; x) = \begin{pmatrix} t & e^T & b^T \\ e & A & B \\ b & B & B \end{pmatrix}, \tag{3.4}$$

where A, B, e, and b are indexed by $V(G) = \mathcal{P}(N)$, $\operatorname{diag}(A) = e$, and $\operatorname{diag}(B) = b$. By Lemma 2.1, we have

$$M_2(\emptyset; x) \succeq 0 \Longleftrightarrow \begin{pmatrix} t-1 & e^T - b^T \\ e-b & A-B \end{pmatrix} \succeq 0 \ \text{ and } \ B \succeq 0. \tag{3.5}$$

As x is invariant under the action of $\operatorname{Aut}(G)$, it follows that $A_{I,J} = x_{\{I,J\}} = x_{\{I',J'\}} = A_{I',J'}$ if $|I \triangle J| = |I' \triangle J'|$. In other words, the matrix A lies in the Bose–Mesner algebra, say,

$$A = \sum_{k=0}^{n} x_k M_k^n = \sum_{i,j,p=0}^{n} x_{i+j-2p} M_{i,j}^{p,n} \tag{3.6}$$

for some reals x_k. Moreover, $B_{I,J} = x_{\{\emptyset,I,J\}} = x_{\{\emptyset,I',J'\}} = B_{I',J'}$ if $|I'| = |I|$, $|J'| = |J|$, and $|I' \cap J'| = |I \cap J|$. In other words, the matrix B lies in the Terwilliger algebra, say,

$$B = \sum_{i,j,p=0}^{n} x_{i,j}^{p} M_{i,j}^{p,n} \tag{3.7}$$

for some reals $x_{i,j}^p$. The following relations link the parameters x_i and $x_{i,j}^p$.

LEMMA 3.4. *For $i, j, p = 0, \ldots, n$,*

$$\begin{aligned} &x_i = x_{0,i}^0, \\ &x_{i,j}^p = x_{j,i}^p = x_{i+j-2p,j}^{j-p} = x_{i+j-2p,i}^{i-p}, \end{aligned} \tag{3.8}$$

and the edge equations read

$$x_{i,j}^p = 0 \quad \text{if} \quad \{i, j, i+j-2p\} \cap \mathcal{D} \neq \emptyset. \tag{3.9}$$

Proof. If $|I| = i$, then $x_i = A_{\emptyset,I} = x_{\{\emptyset,I\}} = B_{\emptyset,I} = x_{0,i}^0$. Let $|I| = i$, $|J| = j$, and $|I \cap J| = p$. Then $x_{i,j}^p = B_{I,J} = B_{J,I} = x_{j,i}^p$. Moreover, $x_{i,j}^p = B_{I,J} = x_{\{\emptyset,I,J\}} = x_{\{I,\emptyset,I\triangle J\}} = B_{I,I\triangle J} = x_{i+j-2p,i}^{i-p}$. This shows (3.8). The edge conditions read $B_{I,J} = x_{\{I,\emptyset,J\}} = 0$ if $\{|I|, |J|, |I \triangle J|\} \cap \mathcal{D} \neq \emptyset$, giving (3.9). ∎

We can now use the results from the previous subsection (Theorem 3.1 and Lemma 3.3) for block-diagonalizing the matrices occurring in (3.5). For $k = 0, \ldots, \lfloor n/2 \rfloor$, define the matrices

$$A_k := \left(\sum_p \alpha_{i,j,k}^{p,n} x_{0,i+j-2p}^0 \right)_{i,j=k}^{n-k}, \qquad B_k := \left(\sum_p \alpha_{i,j,k}^{p,n} x_{i,j}^p \right)_{i,j=k}^{n-k} \tag{3.10}$$

corresponding, respectively, to the matrices A, and B in (3.6) and (3.7). Define the vector

$$\tilde{c} := \left(\sqrt{\binom{n}{i}} \left(1 - x_{0,i}^0\right) \right)_{i=0}^{n} \in \mathbb{R}^{n+1}. \tag{3.11}$$

Then the parameter $\psi(H(n, \mathcal{D}))$ can be reformulated in the following way:

$$\begin{aligned} \psi(H(n,\mathcal{D})) = \min\ t \ \text{ s.t. } \quad & x_{0,0}^0 = 1 \text{ and } x_{i,j}^p \text{ satisfy (3.8) and (3.9), and} \\ & A_k - B_k \succeq 0 \ \text{ for } k = 1, \ldots, \lfloor n/2 \rfloor, \\ & B_k \succeq 0 \ \text{ for } k = 0, 1, \ldots, \lfloor n/2 \rfloor, \\ & \begin{pmatrix} t-1 & \tilde{c}^T \\ \tilde{c} & A_0 - B_0 \end{pmatrix} \succeq 0, \end{aligned} \tag{3.12}$$

where A_k, B_k, and $\tilde{c}$ are as in (3.10) and (3.11). To compute $\psi_{\geq 0}(H(n,\mathcal{D}))$, simply add the nonnegativity condition $x_{i,j}^p \geq 0$ to (3.12).

3.3. Compact formulation for $\Psi_\ell(G)$ for Hamming graphs. We now give a more compact formulation for the parameter $\Psi_\ell(G)$ when $G = H(n,\mathcal{D})$. As mentioned above, one has to evaluate $\ell(G_t)$ for various choices of $t \in \mathbb{N}$, with $\ell(G_t)$ being given by (2.27). As for the parameter $\psi(H(n,\mathcal{D}))$, we now observe that $A^1,\ldots,B^4$, and thus all blocks in the matrices in (2.27) lie in the Terwilliger algebra. (As in the previous section we fix $h := \emptyset$, the empty subset of N.)

LEMMA 3.5. *The matrices A^s $(s = 1,2)$ belong to the Bose–Mesner algebra $\mathcal{B}_n$, and the matrices B^s $(s = 1,2,3,4)$ belong to the Terwilliger algebra $\mathcal{A}_n$, say, $A^s = \sum_{i=0}^n x(s)_i M_i^n$ $(s = 1,2)$ and $B^s = \sum_{i,j,p=0}^n y(s)_{i,j}^p M_{i,j}^{p,n}$ $(s = 1,2,3,4)$. Then*

$$
\begin{gathered}
x(s)_i = y(s)_{0,i}^0 \quad \textit{for } s = 1,2,\ i = 1,\ldots,n,\\
y(s)_{i,j}^p = y(s)_{j,i}^p = y(s)_{i+j-2p,j}^{j-p} = y(s)_{i+j-2p,i}^{i-p} \ (\textit{for } s = 1,4),\\
y(2)_{i,j}^p = y(2)_{i,i+j-2p}^{i-p}, \qquad y(3)_{i,j}^p = y(3)_{j,i}^p,\\
y(3)_{i,j}^p = y(2)_{i+j-2p,i}^{i-p} \quad \textit{for } i,j,p = 0,\ldots,n.
\end{gathered} \tag{3.13}
$$

Moreover, the edge conditions can be reformulated as

$$
\begin{aligned}
&y(1)_{i,j}^p = 0 && \textit{if } \{i,j,i+j-2p\} \cap \mathcal{D} \neq \emptyset,\\
&y(2)_{i,i}^i = y(4)_{i,i}^i = 0 && \textit{for } i = 0,\ldots,n,\\
&y(2)_{i,j}^p = 0 && \textit{if } i \in \mathcal{D} \textit{ or } j = 0,\\
&y(3)_{i,j}^p = 0 && \textit{if } i+j-2p \in \mathcal{D},\ \textit{or } i = 0,\ \textit{or } j = 0,\\
&y(4)_{i,j}^p = 0 && \textit{if } i = 0 \textit{ or } j = 0
\end{aligned} \tag{3.14}
$$

for distinct $i,j \in \{0,1,\ldots,n\}$.

Proof. We use the fact that $A^1,\ldots,B^4$ satisfy (2.24) and (2.25) where the variable y is assumed to be invariant under the action of $\mathrm{Sym}(t) \times \mathrm{Aut}(G) \subseteq \mathrm{Aut}(G_t)$. We have $A^1, A^2 \in \mathcal{B}_n$, since the entries $A_{I,J}^1 = y_{\{1I,1J\}}$ and $A_{I,J}^2 = y_{\{1I,2J\}}$ depend only on $|I \triangle J|$. (Indeed, if $|I' \triangle J'| = |I \triangle J|$, then there exists $\sigma \in \mathrm{Aut}(G)$ mapping $\{I,J\}$ to $\{I',J'\}$, and thus, by the invariance of y under action of σ, $y_{\{1I,1J\}} = y_{\{1I',1J'\}}$ and $y_{\{1I,2J\}} = y_{\{1I',2J'\}}$.) Similarly, for $s = 1,\ldots,4$, $B^s \in \mathcal{A}_n$ since the entry $B_{I,J}^s$ depends only on $|I|, |J|$ and $|I \cap J|$. The proof for the identities $x(s)_i = y(s)_{0,i}^0$ $(s = 1,2)$ and $y(1)_{i,j}^p = \cdots = y(1)_{i+j-2p,i}^{i-p}$ is identical to the proof of (3.8). Let $I,J \in \mathcal{P}(N)$, with $|I| = i$, $|J| = j$, and $|I \cap J| = p$. Then $y(4)_{i,j}^p = B_{I,J}^4 = y_{\{1\emptyset,2I,3J\}} = y_{\{1\emptyset,3I,2J\}}$ (use the invariance of y under the permutation $(2,3) \in \mathrm{Sym}(t)$) and thus is equal to $B_{J,I}^4 = y(4)_{j,i}^p$. Moreover, $y(4)_{i,j}^p = y_{\{1\emptyset,2I,3J\}} = y_{\{1I,2\emptyset,3I\triangle J\}} = y_{\{2I,1\emptyset,3I\triangle J\}}$ (first apply the switching mapping by I and then permute the indices $1,2$) and thus is equal to $B_{I,I\triangle J}^4 = y(4)_{i,i+j-2p}^{i-p}$. Next we have $y(2)_{i,j}^p = B_{I,J}^2 = y_{\{1I,1\emptyset,2J\}} = y_{\{1\emptyset,1I,2I\triangle J\}}$ (apply the switching mapping by I) and thus is equal to $B_{I,I\triangle J}^2 = y(2)_{i,i+j-2p}^{i-p}$. Finally, $y(3)_{i,j}^p = B_{I,J}^3 = y_{\{2I,1\emptyset,2J\}} = B_{J,I}^3 = y(3)_{j,i}^p$, and $y(3)_{i,j}^p = y_{\{2I,1\emptyset,2J\}} = y_{\{2\emptyset,1I,2I\triangle J\}} = y_{\{1\emptyset,2I,1I\triangle J\}}$ (first switch by I and then permute $1,2$) and thus is equal to $B_{I\triangle J,I}^2 = y(2)_{i+j-2p,i}^{i-p}$. The identities (3.14) follow directly from (2.25). $\square$

As the blocks of the matrices in the program (2.27) lie in the Terwilliger algebra, the matrices in (2.27) can be block-diagonalized, as explained in section 3.1. For this, define the matrices

$$A_k^s := \left(\sum_p \alpha_{i,j,k}^{p,n} y(s)_{i+j-2p,0}^0\right)_{i,j=k}^{n-k}, \qquad B_k^s := \left(\sum_p \alpha_{i,j,k}^{p,n} y(s)_{i,j}^p\right)_{i,j=k}^{n-k} \tag{3.15}$$

corresponding, respectively, to the matrices A^s $(s = 1, 2)$ and B^s $(s = 1, 2, 3, 4)$, and define the vectors

(3.16)

$$\tilde{a} := \left(\sqrt{\binom{n}{i}}\left(y(1)_{0,0}^0 - y(1)_{i,i}^i\right)\right)_{i=0}^n, \quad \tilde{b} := \left(\sqrt{\binom{n}{i}}\left(y(1)_{i,i}^i - y(3)_{i,i}^i\right)\right)_{i=0}^n \in \mathbb{R}^{n+1}.$$

By using Lemmas 3.2 and 3.3, we obtain the following reformulation for the parameter $\ell(G_t)$ from (2.27):

(3.17)

$$\ell(G_t) = \max\ 2^n t y(1)_{0,0}^0 \ \text{ s.t. } y(s)_{i,j}^p \ (s = 1, \dots, 4) \text{ satisfy (3.13) and (3.14), and}$$

$$\begin{pmatrix} 1 - y(1)_{0,0}^0 & \tilde{a}^T & (t-1)\tilde{b}^T \\ & A_0^1 - B_0^1 & (t-1)(A_0^2 - B_0^2) \\ & & (t-1)(A_0^1 - B_0^3) + (t-1)(t-2)(A_0^2 - B_0^4) \end{pmatrix} \succeq 0,$$

$$\begin{pmatrix} A_k^1 - B_k^1 & (t-1)(A_k^2 - B_k^2) \\ & (t-1)(A_k^1 - B_k^3) + (t-1)(t-2)(A_k^2 - B_k^4) \end{pmatrix} \succeq 0 \text{ for } k = 1, \dots, \lfloor n/2 \rfloor,$$

$$\begin{pmatrix} B_k^1 & (t-1)B_k^2 \\ & (t-1)B_k^3 + (t-1)(t-2)B_k^4 \end{pmatrix} \succeq 0 \text{ for } k = 0, \dots, \lfloor n/2 \rfloor,$$

$$A_k^1 - A_k^2 - B_k^3 + B_k^4 \succeq 0 \ \text{ for } k = 0, \dots, \lfloor n/2 \rfloor,$$

$$B_k^3 - B_k^4 \succeq 0 \ \text{ for } k = 0, \dots, \lfloor n/2 \rfloor,$$

where A_k^s, B_k^s, $\tilde{a}$, and $\tilde{b}$ are as in (3.15) and (3.16). To compute $\ell_{\geq 0}(G_t)$ simply add the nonnegativity condition $y(s)_{i,j}^p \geq 0$ on all variables.

3.4. Numerical results for Hamming graphs. We have tested the various bounds on some instances of Hamming graphs. In what follows we use the following convention: For an integer $1 \leq d \leq n$, $H(n, d)$ (resp., $H^-(n, d)$, $H^+(n, d)$) denotes the graph $H(n, \mathcal{D})$, with $\mathcal{D} = \{d\}$ (resp., $\mathcal{D} = \{1, \dots, d\}$, $\{d, \dots, n\}$). The papers [9, 10, 11] give numerical results for the parameters $\overline{\vartheta}(G)$ and $\overline{\vartheta^+}(G)$ for such instances. Moreover, a bound related to copositive programming is computed in [11] (called the $\mathcal{K}_1$-bound in [11] or the $\kappa^{(1)}$ bound in [17]); it is shown in [17] that this bound is dominated by our parameter $\psi_{\geq 0}$.

In Table 1, the symbol "*" indicates the strict inequality $\Psi_\ell(G) > \lceil \psi(G) \rceil$, which happens for $H(10, 8)$ and $H^+(10, 8)$, and we indicate in bold the values satisfying LB $= \chi(G)$ for the obtained lower bound (LB). (Indeed, in these instances, LB $= 2^{n-1}$, while $\mathcal{P}(V)$ can be covered by the 2^{n-1} distinct pairs $\{I, V \setminus I\}$ $(I \subseteq V)$ which are stable sets as $n \notin \mathcal{D}$.)

The results in Table 1 indicate that the parameters $\psi(G)$ and $\psi_{\geq 0}(G)$ give in some instances a major improvement on Szegedy's bound $\overline{\vartheta^+}(G)$. On the other hand,

Table 1
Bounds for the chromatic number of Hamming graphs.

Graph	$\overline{\vartheta}(G)$	$\overline{\vartheta^+}(G)$	$\psi(G)$	$\Psi_\ell(G)$	$\psi_{\geq 0}(G)$	$\Psi_{\ell_{\geq 0}}(G)$
$H^-(7,4)$	36	42.6667	**64**	**64**	**64**	**64**
$H^-(8,5)$	72	85.3333	**128**	**128**	**128**	**128**
$H(10,6)$	6	8.7273	10.4366	11	10.8936	11
$H^-(10,6)$	207.36	320	**512**	**512**	**512**	**512**
$H(10,8)$	2.6667	3.2	3.9232	5*	3.9232	5*
$H^+(10,8)$	3.2	3.2	3.9232	5*	3.9232	5*
$H(11,4)$	16	21.5652	25.7351	26	25.7351	26
$H(11,6)$	12	12	12	12	15.2836	16
$H^-(11,7)$	414.72	640	**1024**	**1024**	**1024**	**1024**
$H^-(11,8)$	711.1111	819.2	**1024**	**1024**	**1024**	**1024**
$H(11,8)$	3.2	4.9383	5.7805	6	5.7805	6
$H(13,8)$	5.3333	9.4118	12.1429	13	13.6533	14
$H(15,6)$	27.7647	30.7368	46.4371	47	50.3036	51
$H(16,8)$	16	16	16	16	28.4444	29
$H(17,6)$	35	48.2222	86.3086	87	88.3204	89
$H(17,8)$	18	18	32	32	46.5122	47
$H(17,10)$	6.6666	12.6315	15.8750	16	25.8405	26
$H(18,10)$	10	16	18.3076	19	38.8844	-
$H(20,6)$	59.3735	59.3735	140.9586	141	140.9586	-
$H(20,8)$	41.7143	60.9524	107.1489	-	136.4115	-

in most cases, the parameter $\Psi_\ell(G)$ gives no improvement since $\Psi_\ell(G) = \lceil \psi(G) \rceil$. It could be that this feature is specific to Hamming graphs. As we will see in the next section, the bound $\Psi_\ell(G)$ does improve the bound $\lceil \psi(G) \rceil$ for Kneser graphs.

4. Bounds for Kneser graphs. We have seen that the parameter $\psi(G)$ is bounded by $\chi^*(G)$ and that, for vertex-transitive graphs, it coincides with the bound $|V(G)|/\ell(G)$. On the other hand, $\Psi_\ell(G)$ can sometimes be strictly greater than $\lceil \psi(G) \rceil$, e.g., for the Hamming graph $H(10,8)$ (recall Table 1). We present here some numerical results showing that $\Psi_\ell(G)$ can in fact be strictly greater than $\lceil \chi^*(G) \rceil$ for Kneser graphs.

Given integers $n \geq 2r$, the Kneser graph $K(n,r)$ is the graph whose vertices are the subsets of size r of a set N, with $|N| = n$, two vertices being adjacent if and only if they are disjoint. As shown in [24], $\alpha(K(n,r)) = \binom{n-1}{r-1}$, and thus $\chi^*(K(n,r)) = \frac{n}{r}$ in view of (2.2) as $K(n,r)$ is vertex-transitive. Lovász proved that $\chi(K(n,r)) = n-2r+2$ in his celebrated paper [23]. Thus the fractional chromatic number and the chromatic number of $K(n,r)$ can differ significantly, while the fractional chromatic number is close to the clique number $\omega(K(n,r)) = \lfloor \frac{n}{r} \rfloor$. Moreover, Lovász [24] proved that, for $G = K(n,r)$, $\alpha(G) = \vartheta(G)$. Hence, $\ell(G) = \alpha(G)$, implying that $\psi(G) = \frac{|V(G)|}{\ell(G)} = \chi^*(G) = n/r$. Therefore, $\Psi_\ell(G) \geq \lceil n/r \rceil$. We show in this section how to compute $\Psi_\ell(G)$.

The Kneser graph $K(n,r)$ coincides with the subgraph of the Hamming graph $H(n,\{2r\})$ induced by the subset $\mathcal{P}_{=r}(N) := \{I \in \mathcal{P}(N) \mid |I| = r\}$. It will be convenient to view the Kneser graph also in the following alternative way. Fix a set $T \subseteq N$, with $|T| = r$, and define

$$\mathcal{P}(N,T) := \{(I', I'') \in \mathcal{P}(T) \times \mathcal{P}(N \setminus T) \mid |I'| = |I''|\}.$$

The mapping

$$\begin{array}{ccc} \mathcal{P}_{=r}(N) & \longrightarrow & \mathcal{P}(N,T), \\ I & \mapsto & (T \setminus I, I \setminus T) \end{array} \tag{4.1}$$

is a bijection, and $|I \triangle J| = |(T\setminus I)\triangle(T\setminus J)|+|(I\setminus T)\triangle(J\setminus T)|$ holds for $I, J \in \mathcal{P}_{=r}(N)$. Hence $K(n,r)$ can also be viewed as the graph with node set $\mathcal{P}(N,T)$, with two nodes $(I', I''), (J', J'') \in \mathcal{P}(N,T)$ being adjacent if $|I' \triangle J'| + |I'' \triangle J''| = 2r$.

As we will see below, the matrices involved in the program (2.27) for the computation of $\Psi_\ell(K(n,r))$ lie in $\mathcal{B}_{r,r'}$ ($r' = n-r$), a subalgebra of a tensor product of two Terwilliger algebras, which has also been studied and block-diagonalized by Schrijver [31] (in connection with constant-weight codes). We follow the same steps as in section 3 for the computation of $\ell(G_t)$ for Hamming graphs, which we now carry out for Kneser graphs.

4.1. The subalgebra $\boldsymbol{\mathcal{B}_{r,r'}}$. As above, $|N| = n$, and we fix a subset $T \subseteq N$, with $|T| = r$, and set $r' := n - r$. For $i, j, p = 0, 1, \dots, r$ (resp., $i', j', q = 0, 1, \dots, r'$), let $M^{p,r}_{i,j}$ (resp., $M^{q,r'}_{i',j'}$) be the matrices indexed by $\mathcal{P}(T)$ (resp., $\mathcal{P}(N \setminus T)$) defining the Terwilliger algebra $\mathcal{A}_r$ (resp., $\mathcal{A}_{r'}$) as in section 3.1. Let now $\mathcal{A}_{r,r'}$ be the algebra generated by the tensor products of matrices in $\mathcal{A}_r$ and $\mathcal{A}_{r'}$, that is,

$$\mathcal{A}_{r,r'} := \left\{ \sum_{i,j,p,i',j',q} x^{p,q}_{i,j,i',j'} M^{p,r}_{i,j} \otimes M^{q,r'}_{i',j'} \mid x^{p,q}_{i,j,i',j'} \in \mathbb{R} \right\}.$$

Matrices in $\mathcal{A}_{r,r'}$ are indexed by the set $\mathcal{P}(T) \times \mathcal{P}(N \setminus T)$. Consider the subalgebra

$$\mathcal{B}_{r,r'} := \left\{ \sum_{i,j,p,q} y^{p,q}_{i,j} M^{p,r}_{i,j} \otimes M^{q,r'}_{i,j} \mid y^{p,q}_{i,j} \in \mathbb{R} \right\}.$$

So $\mathcal{B}_{r,r'}$ consists of all matrices from $\mathcal{A}_{r,r'}$ satisfying $x^{p,q}_{i,j,i',j'} = 0$ if $i \neq i'$ or $j \neq j'$. Hence, for $M \in \mathcal{B}_{r,r'}$ and $(I, I'), (J, J') \in \mathcal{P}(T) \times \mathcal{P}(N \setminus T)$, $M_{(I,I'),(J,J')} = 0$ if $|I| \neq |I'|$ or if $|J| \neq |J'|$. Therefore any row/column of M indexed by $(I, I') \notin \mathcal{P}(N,T)$ is identically zero, and we may thus restrict matrices in $\mathcal{B}_{r,r'}$ to being indexed by the subset $\mathcal{P}(N,T)$ of $\mathcal{P}(T) \times \mathcal{P}(N \setminus T)$.

For $k \leq r$, let $M^{n,r}_k$ be the matrix indexed by $\mathcal{P}(N,T)$, whose $((I,I'),(J,J'))$th entry is equal to 1 if $|I \triangle J|+|I' \triangle J'| = 2k$ and to 0 otherwise. Thus $M^{n,r}_k$ corresponds to the principal submatrix of M^n_{2k} (in the Bose–Mesner algebra $\mathcal{B}_n$) indexed by the subset $\mathcal{P}_{=r}(N)$ and $M^{n,r}_k \in \mathcal{B}_{r,r'}$ as $M^{n,r}_k = \sum_{i,j,p,q \mid i+j-p-q=k} M^{p,r}_{i,j} \otimes M^{q,r'}_{i,j}$. Hence the set

$$\mathcal{B}^r_n := \left\{ \sum_{k=0}^{r} x_k M^{n,r}_k \mid x_k \in \mathbb{R} \right\}$$

is a subalgebra of $\mathcal{B}_{r,r'}$.

Schrijver [31] proved the following analogue of Theorem 3.1, giving the explicit block-diagonalization for matrices in $\mathcal{B}_{r,r'}$. For $k = 0, \dots, \lfloor \frac{r}{2} \rfloor$, $l = 0, \dots, \lfloor \frac{r'}{2} \rfloor$, set

$$W_{kl} := \{k, k+1, \dots, r-k\} \cap \{l, l+1, \dots, r'-l\}.$$

THEOREM 4.1 (see [31]). *For a matrix* $M = \sum_{i,j,p,q} y^{p,q}_{i,j} M^{p,r}_{i,j} \otimes M^{q,r'}_{i,j}$ *in* $\mathcal{B}_{r,r'}$,

$$M \succeq 0 \iff M_{k,l} := \left(\sum_{p,q} \alpha^{p,r}_{i,j,k} \alpha^{q,r'}_{i,j,l} y^{p,q}_{i,j} \right)_{i,j \in W_{kl}} \succeq 0 \tag{4.2}$$
$$\text{for each } k = 0, 1, \dots, \left\lfloor \tfrac{r}{2} \right\rfloor \text{ and } l = 0, 1, \dots, \left\lfloor \tfrac{r'}{2} \right\rfloor.$$

We have the following analogues of Lemmas 3.2 and 3.3.

LEMMA 4.2. *Let* $A = \sum_{i,j,p,q} a_{i,j}^{p,q} M_{i,j}^{p,r} \otimes M_{i,j}^{q,r'}$, $B = \sum_{i,j,p,q} b_{i,j}^{p,q} M_{i,j}^{p,r} \otimes M_{i,j}^{q,r'}$, *and* $C = \sum_{i,j,p,q} c_{i,j}^{p,q} M_{i,j}^{p,r} \otimes M_{i,j}^{q,r'}$ *be matrices in* $\mathcal{B}_{r,r'}$, *and define accordingly*

$$A_{kl} = \left(\sum_{p,q} \alpha_{i,j,k}^{p,r} \alpha_{i,j,l}^{q,r'} a_{i,j}^{p,q}\right)_{i,j \in W_{kl}}, \qquad B_{kl} = \left(\sum_{p,q} \alpha_{i,j,k}^{p,r} \alpha_{i,j,l}^{q,r'} b_{i,j}^{p,q}\right)_{i,j \in W_{kl}},$$

$$C_{kl} = \left(\sum_{p,q} \alpha_{i,j,k}^{p,r} \alpha_{i,j,l}^{q,r'} c_{i,j}^{p,q}\right)_{i,j \in W_{kl}}.$$

Then

$$\begin{pmatrix} A & B \\ B^T & C \end{pmatrix} \succeq 0 \Longleftrightarrow \begin{pmatrix} A_{kl} & B_{kl} \\ B_{kl}^T & C_{kl} \end{pmatrix} \succeq 0 \ \forall k = 0, 1, \ldots, \left\lfloor \frac{r}{2} \right\rfloor \text{ and } l = 0, 1, \ldots, \left\lfloor \frac{r'}{2} \right\rfloor.$$

LEMMA 4.3. *Let* $M = \sum_{i,j,p,q=0}^{n} x_{i,j}^{p,q} M_{i,j}^{p,r} \otimes M_{i,j}^{q,r'} \in \mathcal{B}_{r,r'}$ *and* $c = \sum_{i=0}^{n} c_i \chi^i$, *where* $\chi^i \in \{0,1\}^{\mathcal{P}(N,T)}$ *with* $\chi^i_{(I,I')} = 1$ *if* $|I| = i$ *(for* $(I, I') \in \mathcal{P}(N,T)$*) and* $d \in \mathbb{R}$. *Then*

$$\begin{pmatrix} d & c^T \\ c & M \end{pmatrix} \succeq 0 \Longleftrightarrow \begin{cases} M_{kl} \succeq 0 \ \text{ for } k = 0, \ldots, \left\lfloor \frac{r}{2} \right\rfloor, l = 0, \ \ldots, \left\lfloor \frac{r'}{2} \right\rfloor, \ k + l > 0; \\ \tilde{M}_{00} := \begin{pmatrix} d & \tilde{c}^T \\ \tilde{c} & M_{00} \end{pmatrix} \succeq 0 \end{cases}$$

after setting $\tilde{c}^T := (c_i \sqrt{\binom{r}{i}\binom{r'}{i}})_{i=0}^{r}$.

4.2. Compact formulation for $\Psi_\ell(G)$ for Kneser graphs. In order to compute $\Psi_\ell(G)$ for the Kneser graph $G = K(n,r)$, one has to evaluate $\ell(G_t)$ for various choices of t. As G is vertex-transitive, $\ell(G_t)$ can be computed by using the program (2.27). We now fix $h := T \in \mathcal{P}_{=r}(N)$ corresponding to $(\emptyset, \emptyset) \in \mathcal{P}(N,T)$ as a chosen node of G. We now show that the matrices $A^1, \ldots, B^4$ appearing in program (2.27) lie in the algebra $\mathcal{B}_{r,r'}$, and thus they can be block-diagonalized by using Theorem 4.1. The following lemma is the analogue of Lemma 3.5.

LEMMA 4.4. *The matrices* A^s $(s = 1, 2)$ *belong to* $\mathcal{B}_n^r$, *and the matrices* B^s $(s = 1, 2, 3, 4)$ *belong to* $\mathcal{B}_{r,r'}$, *say,* $A^s = \sum_{i=0}^{r} x(s)_i M_i^{n,r}$ $(s = 1, 2)$ *and* $B^s = \sum_{i,j,p,q=0}^{r} y(s)_{i,j}^{p,q} M_{i,j}^{t,r} \otimes M_{i,j}^{q,r'}$ $(s = 1, 2, 3, 4)$. *We have*

$$\begin{aligned} x(s)_i &= y(s)_{0,i}^{0,0} \quad \text{for } s = 1, 2, \ i = 1, \ldots, r, \\ y(s)_{i,j}^{p,q} = y(s)_{j,i}^{p,q} &= y(s)_{i,i+j-p-q}^{i-q,i-p} = y_{j,i+j-p-q}^{j-q,j-p} \quad \text{for } s = 1, 4, \\ y(2)_{i,j}^{p,q} &= y(2)_{i,i+j-p-q}^{i-q,i-p}, \qquad y(3)_{i,j}^{p,q} = y(3)_{j,i}^{p,q}, \\ y(3)_{i,j}^{p,q} &= y(2)_{i+j-p-q,i}^{i-q,i-p} \quad \text{for } i, j, p, q = 0, \ldots, r. \end{aligned} \tag{4.3}$$

Moreover, the edge conditions can be reformulated as

$$\begin{aligned} y(1)_{i,j}^{p,q} &= 0 \quad \text{if } \ i = r, \ \text{ or } j = r, \ \text{ or } i + j - p - q = r, \\ y(2)_{i,j}^{p,q} &= 0 \quad \text{if } i = r, \ \text{ or } j = 0, \ \text{ or } i + j - p - q = 0, \\ y(3)_{i,j}^{p,q} &= 0 \quad \text{if } i = 0, \ \text{ or } j = 0, \ \text{ or } i + j - p - q = r, \\ y(4)_{i,j}^{p,q} &= 0 \quad \text{if } i = 0, \ \text{ or } j = 0, \ \text{ or } i + j - p - q = 0. \end{aligned} \tag{4.4}$$

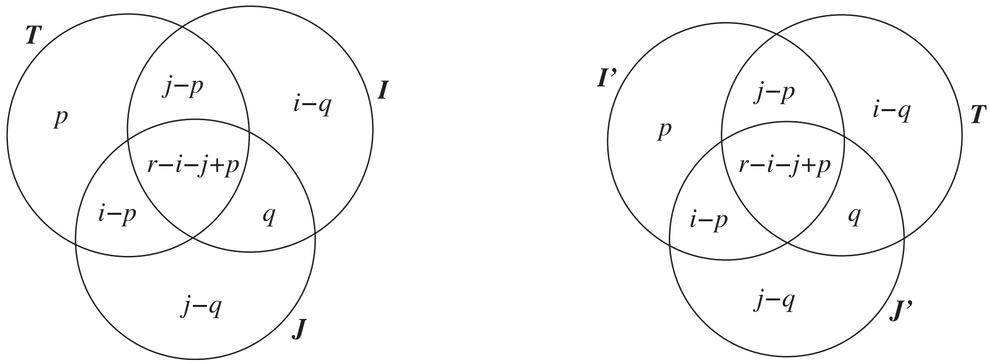

FIG. 4.1. *Venn diagrams.*

Proof. As in the proof of Lemma 3.5, the matrices $A^1, \ldots, B^4$ satisfy (2.24) and (2.25), where the variable y is invariant under the action of $\mathrm{Sym}(t) \times \mathrm{Aut}(G)$. A main difference with the case of the Hamming graph is that, for the Kneser graph $G = K(n, r)$, $\mathrm{Aut}(G) \sim \mathrm{Sym}(n)$; i.e., the only automorphisms of G arise from the permutations of N. Recall that $\sigma \in \mathrm{Sym}(n)$ acts on $\mathcal{P}_{=r}(N)$ in the obvious way, by letting $\sigma(I) = \{\sigma(i) \mid i \in I\}$ for $I \in \mathcal{P}_{=r}(N)$.

Let us first show that $A^1 \in \mathcal{B}_n^r$; that is, $A^1_{I,J}$ depends only on $|I \bigtriangleup J|$ (for $I, J \in \mathcal{P}_{=r}(N)$). For this, let $I, J, I', J' \in \mathcal{P}_{=r}(N)$, with $|I \bigtriangleup J| = |I' \bigtriangleup J'|$. Then $|I \cap J| = |I' \cap J'|$, and thus there exists $\sigma \in \mathrm{Sym}(n)$ such that $\sigma(I) = I'$ and $\sigma(J) = J'$. Hence, $A^1_{I,J} = y_{\{1I,1J\}} = y_{\{1\sigma(I),1\sigma(J)\}} = A^1_{I',J'}$ since y is invariant under the action of σ. The proof for $A^2 \in \mathcal{B}_n^r$, $B^s \in \mathcal{B}_{r,r'}$, is along the same lines.

Let us now prove the identity $y(1)^{p,q}_{i,j} = y(1)^{i-q,i-p}_{i,i+j-p-q}$; the proofs for the remaining identities are along the same lines and thus are omitted. Say, $y(1)^{p,q}_{i,j} = B^1_{I,J}$, where $I, J \in \mathcal{P}_{=r}(N)$ with $|T \setminus I| = i$, $|T \setminus J| = j$, $|(T \setminus I) \cap (T \setminus J)| = p$, and $|(I \setminus T) \cap (J \setminus T)| = q$. See Figure 4.1 for the Venn diagram of the sets I, J, and T. Consider sets $I', J' \in \mathcal{P}_{=r}(N)$, which together with the set T have the Venn diagram shown in Figure 4.1. Then $B^1_{I',J'} = y(1)^{i-q,i-p}_{i,i+j-p-q}$, and there exists $\sigma \in \mathrm{Sym}(n)$ such that $\sigma(T) = I'$, $\sigma(I) = T$, and $\sigma(J) = J'$. Therefore, $y(1)^{p,q}_{i,j} = B^1_{I,J} = y_{\{1I,1J,1T\}} = y_{\{1\sigma(I),1\sigma(J),1\sigma(T)\}} = y_{\{1T,1J',1I'\}} = B^1_{I',J'} = y(1)^{i-q,i-p}_{i,i+j-p-q}$. ∎

For $k = 0, \ldots, \lfloor r/2 \rfloor$, $l = 0, \ldots, \lfloor r'/2 \rfloor$, define the matrices

(4.5)
$$A^s_{kl} = \left(\sum_{p,q} \alpha^{p,r}_{i,j,k} \alpha^{q,r'}_{i,j,l} y(s)^{0,0}_{0,i+j-p-q} \right)_{i,j \in W_{kl}}, \qquad B^s_{kl} = \left(\sum_{p,q} \alpha^{p,r}_{i,j,k} \alpha^{q,r'}_{i,j,l} y(s)^{p,q}_{i,j} \right)_{i,j \in W_{kl}}$$

corresponding, respectively, to the matrices A^s ($s = 1, 2$) and B^s ($s = 1, 2, 3, 4$), and define the vectors

(4.6)
$$\tilde{a} := \left(\sqrt{\binom{r}{i}\binom{r'}{i}} \left(y(1)^{0,0}_{0,0} - y(1)^{i,i}_{i,i} \right) \right)_{i=0}^{r}, \qquad \tilde{b} := \left(\sqrt{\binom{r}{i}\binom{r'}{i}} \left(y(1)^{i,i}_{i,i} - y(3)^{i,i}_{i,i} \right) \right)_{i=0}^{r}.$$

By using Lemmas 4.2 and 4.3, we obtain the following reformulation for the parameter

$\ell(G_t)$ from (2.27):

(4.7)

$$\ell(G_t) = \max \binom{n}{r} t y(1)^{0,0}_{0,0} \text{ s.t. } y(s)^{p,q}_{i,j},\ s = 1,\dots,4 \text{ satisfy (4.3) and (4.4), and}$$

$$\begin{pmatrix} 1 - y(1)^{0,0}_{0,0} & \tilde{a}^T & (t-1)\tilde{b}^T \\ & A^1_{00} - B^1_{00} & (t-1)(A^2_{00} - B^2_{00}) \\ & & (t-1)(A^1_{00} - B^3_{00}) + (t-1)(t-2)(A^2_{00} - B^4_{00}) \end{pmatrix} \succeq 0;$$

$$\begin{pmatrix} A^1_{kl} - B^1_{kl} & (t-1)(A^2_{kl} - B^2_{kl}) \\ & (t-1)(A^1_{kl} - B^3_{kl}) + (t-1)(t-2)(A^2_{kl} - B^4_{kl}) \end{pmatrix} \succeq 0$$
$$\text{for } k = 0,\dots,\lfloor r/2 \rfloor, l = 0,\dots,\lfloor r'/2 \rfloor,\ k + l > 0;$$

$$\begin{pmatrix} B^1_{kl} & (t-1)B^2_{kl} \\ & (t-1)B^3_{kl} + (t-1)(t-2)B^4_{kl} \end{pmatrix} \succeq 0 \text{ for } k = 0,\dots,\lfloor r/2 \rfloor, l = 0,\dots,\lfloor r'/2 \rfloor;$$

$$A^1_{kl} - A^2_{kl} - B^3_{kl} + B^4_{kl} \succeq 0 \ \text{ for } k = 0,\dots,\lfloor r/2 \rfloor, l = 0,\dots,\lfloor r'/2 \rfloor;$$

$$B^3_{kl} - B^4_{kl} \succeq 0 \ \text{ for } k = 0,\dots,\lfloor r/2 \rfloor, l = 0,\dots,\lfloor r'/2 \rfloor,$$

where A^s_{kl}, B^s_{kl}, $\tilde{a}$, and $\tilde{b}$ are as in (4.5) and (4.6). To compute $\ell_{\geq 0}(G_t)$ simply add the nonnegativity condition $y(s)^{p,q}_{i,j} \geq 0$ on all variables.

4.3. Numerical results for Kneser graphs. We show in Table 2 below our numerical results for the bounds $\Psi_\ell(G)$ and $\Psi_{\ell_{\geq 0}}(G)$ for several instances of Kneser graphs. We indicate in bold the values achieving the chromatic number.

5. Computing the new bound ψ_K for DIMACS benchmark graphs.

So far we have been dealing with vertex-transitive graphs and with the bounds $\psi(\cdot)$ and $\Psi_\ell(\cdot)$. For the formulation of $\psi(G)$, it was observed in section 2 that, when G is vertex-transitive, it suffices to require in (2.13) positive semidefiniteness of $M_2(h, x)$ for *only one* $h \in V(G)$ instead of *for all* $h \in V(G)$. In the case of a nonsymmetric graph G one would need to require $M_2(h, x) \succeq 0$ for *all* $h \in V(G)$; therefore, with

TABLE 2
Bounds for the chromatic number of Kneser graphs.

Graph	$\lceil \chi^*(G) \rceil = \lceil n/r \rceil$	$\Psi_\ell(G)$	$\Psi_{\ell_{\geq 0}}(G)$	$\chi(G) = n - 2r + 2$
$K(6,2)$	3	**4**	**4**	**4**
$K(7,2)$	4	4	**5**	**5**
$K(8,3)$	3	**4**	**4**	**4**
$K(9,3)$	3	4	4	5
$K(10,4)$	3	3	**4**	**4**
$K(11,3)$	4	5	5	7
$K(11,4)$	3	4	4	5
$K(12,3)$	4	5	6	8
$K(12,4)$	3	4	4	6
$K(12,5)$	3	3	**4**	**4**
$K(13,5)$	3	4	4	5
$K(14,5)$	3	4	4	6
$K(15,3)$	5	6	6	11
$K(16,4)$	4	5	6	10
$K(24,6)$	4	4	6	14
$K(25,5)$	5	6	7	17
$K(34,7)$	5	6	7	22
$K(36,6)$	6	7	9	26

$n := |V(G)|$, in order to compute $\psi(G)$ (resp., $\ell(G_t)$, and thus $\Psi_\ell(G)$), one would have to solve a semidefinite program with $2n$ (resp., $4n$) matrices of order $\leq n+1$ (resp., $\leq 2n+1$). For graphs that are of interest, e.g., with $n \geq 100$, this cannot be done with the currently available software for semidefinite programming.

For nonsymmetric graphs we propose another variant of the bound $\psi^{(2)}(G)$. Given a clique K in G, let $M_2(K;x)$ denote the principal submatrix of $M_2(x)$ indexed by the multiset $\mathcal{P}_1(V) \cup (\cup_{h\in K}\{\{h,i\} \mid i \in V\})$. Now define the parameter

$$\psi_K(G) := \min\ t \ \text{ s.t. } \quad \begin{array}{l} x_{\mathbf{0}} = t,\ x_i = 1\ (i \in V),\ M_2(K;x) \succeq 0, \\ x_I = 0 \text{ for all } I \text{ containing an edge.} \end{array} \tag{5.1}$$

Then $\overline{\vartheta}(G) \leq \psi_K(G) \leq \chi^*(G)$. (The left inequality follows by using (2.4), and the right inequality follows from $\psi_K(G) \leq \psi^{(2)}(G) \leq \chi^*(G)$ by using (2.8) and (2.10).) Set $k := |K|$, and assume without loss of generality that $K = \{1, 2, \ldots, k\}$. With respect to the partition of its index set as $\{\mathbf{0}\} \cup \{\{i\} \mid i \in V\} \cup \cup_{h=1}^{k}\{\{h,i\} \mid i \in V\}$, the matrix $M_2(K;x)$ has the block form

$$M_2(K;x) = \begin{pmatrix} t & a_0^T & a_1^T & a_2^T & \ldots & a_k^T \\ a_0 & A_0 & A_1 & A_2 & \ldots & A_k \\ a_1 & A_1 & A_1 & 0 & \ldots & 0 \\ a_2 & A_2 & 0 & A_2 & \ddots & \vdots \\ \vdots & \vdots & \vdots & \ddots & \ddots & 0 \\ a_k & A_k & 0 & \ldots & 0 & A_k \end{pmatrix},$$

where $a_0, \ldots, a_k, A_0, \ldots, A_k$ are indexed by V, $a_i = \mathrm{diag}(A_i)$ $(0 \leq i \leq k)$, $a_0 = e$, $(A_0)_{ij} = x_{ij}$, and $(A_h)_{ij} = x_{\{h,i,j\}}$ for $h \in K$, $i,j \in V$. Note that for $h \in V$ the columns of A_0 and A_h indexed by $\{h\}$ are both equal to a_h. Hence, as in the proof of Lemma 2.1, we can do some row/column manipulations and verify that

$$M_2(K;x) \succeq 0 \Longleftrightarrow \begin{pmatrix} t-k & e^T - (\sum_{h=1}^k a_h)^T \\ e - \sum_{h=1}^k a_h & A_0 - \sum_{h=1}^k A_h \end{pmatrix} \succeq 0, \quad A_1, \ldots, A_k \succeq 0.$$

Hence $\psi_K(G)$ can be computed via a semidefinite program involving $k+1$ matrices of sizes $n+1$ (once) and n (k times).

We have conducted experiments for some DIMACS benchmark graphs (studied, e.g., in [4, 5, 8, 9, 12, 26, 27]). In Table 3 we present our lower bounds for the chromatic number of the graphs DSJC$a.b$. Recall that DSJC$a.b$ are random graphs with a vertices, two vertices being adjacent with probability $10^{-1}b$. The graph DSJR500.1 is a geometric graph with 500 nodes randomly distributed in the unit square, with an edge between two nodes if their distance is less than 0.1. The graph DSJR500.1c is the complement of DSJR500.1. The graphs can be downloaded from [34].

In Table 3, the column "LB" contains the previously best known lower bounds taken from [8, 26, 27], and the values in parentheses come from [3]; the bound 82 for DSJR500.1c is the size of a clique obtained by using the heuristic of [2]. The column "UB" contains the best known upper bounds taken from [4, 12, 13], i.e., the number of colors in the best colorings found so far. The column "K" contains the size of the clique used for computing the parameter $\psi_K(G)$ (the clique is found by using the heuristic from [2]). We also indicate the value of the theta number $\overline{\vartheta}(G)$ (also computed in [9, 10] for some instances), which already improves the best lower bound

Table 3
Bounds for the chromatic number of DIMACS instances.

Graph	LB	$\overline{\vartheta}(G)$	$\lceil\overline{\vartheta}(G)\rceil$	K	$\psi_K(G)$	$\lceil\psi_K(G)\rceil$	UB
DSJC125.1	5	4.1062	5	4	4.337	**5**	5
DSJC125.5	14 (17)	11.7844	12	10	13.942	**14**	17
DSJC125.9	42	37.768	38	34	42.53	**43**	43
DSJC250.1	6 (8)	4.906	5	4	5.208	**6**	8
DSJC250.5	14	16.234	17	12	19.208	**20**	28
DSJC250.9	48	55.152	56	43	66.15	**67**	72
DSJC500.1	6	6.217	**7**	5	6.542	7	12
DSJC500.5	13 (16)	20.542	21	13	27.791	**28**	48
DSJC500.9	59	84.04	85	56	100.43	**101**	126
DSJC1000.1	6	8.307	**9**	5	-	-	20
DSJC1000.5	15 (17)	31.89	**32**	14	-	-	83
DSJC1000.9	66	122.67	**123**	65	-	-	224
DSJR500.1c	82 (83)	83.74	84	77	84.12	**85**	85

in several instances. We indicate in bold our best new lower bounds for the chromatic number. In several instances they give a significant improvement on the best known lower bound. Moreover, in two instances, we are able to close the gap as our lower bound matches the upper bound; indeed we find the exact value of the chromatic number for the graphs DSJC125.9 ($\chi(G) = 43$) and DSJR500.1c ($\chi(G) = 85$), which were not known before to the best of our knowledge. These results demonstrate that the bounds $\psi_K(G)$ can be quite strong.

One may wonder why we did not add nonnegativity constraints in the formulation for ψ_K. The reason is that for random graphs adding nonnegativity constraints gives only a negligible improvement. This fact was already observed for the Lovász theta number in [9].

Remarks about the computational results. The computational results reported in Tables 1 and 2 were carried out by using the open source codes for semidefinite programming CSDP 5.0 and DSDP 5.8 available, respectively, at [35] and [36].

For finding the large cliques reported in column "K" of Table 3, we used the heuristic Max-AO (based on [2]), available at [37]. The values in the columns "$\overline{\vartheta}(G)$" and "$\psi_K(G)$" of Table 3 were computed by using the boundary point method of Povh, Rendl, and Wiegele [29], whose code is available at [38].

The semidefinite program for the parameter ψ_K can indeed be quite large. For instance, for the graph DSJR500.1*c*, it contains one 501×501 block and 77 blocks of size at most 500×500, and such a big problem cannot be solved by using solvers based on interior point methods.

Experiments were conducted on a single machine with an AMD Athlon 64 3500 processor and 1024 MB RAM memory. Here is a rough indication of the times needed to compute the bounds in Tables 1–3. Each bound in Tables 1–2 could be computed in less than a minute, as it involves a relatively small SDP; for instance, computing $\Psi_\ell(H(20,6))$ is via an SDP with 1502 variables and 47 blocks with sizes ranging from 1 to 43. It was harder to compute the bounds ψ_K in Table 3. In fact, we had to rerun the boundary point code several times for each instance in order to tailor the parameters of the code and speed up the convergence to an optimal solution. The computation times for the parameter $\psi_K(G)$ vary from a few minutes (e.g., less than 3 minutes for DCJC125.5 and about 25 minutes for DCJC125.1) up to four days for the most demanding instance DSJR500.1c.

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